

result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 18:01:10 ON 08 FEB 2007

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CAPLUS' ENTERED AT 18:01:21 ON 08 FEB 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 8 Feb 2007 VOL 146 ISS 7

FILE LAST UPDATED: 7 Feb 2007 (20070207/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 3,4-dihydroxy phenylalanines

6811502 3

5516978 4

86769 DIHYDROXY

1 DIHYDROXIES

86770 DIHYDROXY

(DIHYDROXY OR DIHYDROXIES)

776 PHENYLALANINES

L1 0 3,4-DIHYDROXY PHENYLALANINES

(3 (W) 4 (W) DIHYDROXY (W) PHENYLALANINES)

=> s phenylalanine

79334 PHENYLALANINE

776 PHENYLALANINES

L2 79646 PHENYLALANINE

(PHENYLALANINE OR PHENYLALANINES)

=> s deuterated

L3 32116 DEUTERATED

=> s L2 and L3

L4 234 L2 AND L3

=> s deuterated phenylalanine

32116 DEUTERATED

79334 PHENYLALANINE

776 PHENYLALANINES

79646 PHENYLALANINE

(PHENYLALANINE OR PHENYLALANINES)

L5 48 DEUTERATED PHENYLALANINE

(DEUTERATED (W) PHENYLALANINE)

=> d L5 1-48 bib abs

L5 ANSWER 1 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2006:834575 CAPLUS  
DN 145:371664  
TI Insights into the Catalytic Mechanisms of Phenylalanine and Tryptophan  
Hydroxylase from Kinetic Isotope Effects on Aromatic Hydroxylation  
AU Pavon, Jorge Alex; Fitzpatrick, Paul F.  
CS Department of Biochemistry and Biophysics and Department of Chemistry,  
Texas A&M University, College Station, TX, 77843-2128, USA  
SO Biochemistry (2006), 45(36), 11030-11037  
CODEN: BICHAW; ISSN: 0006-2960  
PB American Chemical Society  
DT Journal  
LA English  
AB Phenylalanine hydroxylase (PheH) and tryptophan hydroxylase (TrpH)  
catalyze the aromatic hydroxylation of phenylalanine and tryptophan, forming  
tyrosine and 5-hydroxytryptophan, resp. The reactions of PheH and TrpH  
have been investigated with [4-2H]-, [3,5-2H2]-, and 2H5-phenylalanine as  
substrates. All Dkcat values are normal with  $\Delta 117$ PheH, the  
catalytic core of rat phenylalanine hydroxylase, ranging from 1.12-1.41.  
In contrast, for  $\Delta 117$ PheH V379D, a mutant protein in which the  
stoichiometry between tetrahydropterin oxidation and amino acid hydroxylation  
is altered, the Dkcat value with [4-2H]-phenylalanine is 0.92 but is  
normal with [3,5-2H2]-phenylalanine. The ratio of tetrahydropterin oxidation  
to amino acid hydroxylation for  $\Delta 117$ PheH V379D shows a similar  
inverse isotope effect with [4-2H]-phenylalanine. Intramol. isotope  
effects, determined from the deuterium contents of the tyrosine formed from  
[4-2H]- and [3,5-2H2]-phenylalanine, are identical for  $\Delta 117$ PheH and  
 $\Delta 117$ PheH V379D, suggesting that steps subsequent to oxygen addition are  
unaffected in the mutant protein. The inverse effects are consistent with  
the reaction of an activated ferryl-oxo species at the para position of  
the side chain of the amino acid to form a cationic intermediate. The  
normal effects on the Dkcat value for the wild-type enzyme are attributed  
to an isotope effect of 5.1 on the tautomerization of a dienone  
intermediate to tyrosine with a rate constant 6- to 7-fold that for  
hydroxylation. In addition, there is a slight (.apprx.34%) preference for  
the loss of the hydrogen originally at C4 of phenylalanine. With  
2H5-indole-tryptophan as a substrate for  $\Delta 117$ PheH, the Dkcat value  
is 0.89, consistent with hydroxylation being rate-limiting in this case.  
When deuterated phenylalanines are used as substrates  
for TrpH, the Dkcat values are within error of those for  $\Delta 117$ PheH  
V379D. Overall, these results are consistent with the aromatic amino acid  
hydroxylases all sharing the same chemical mechanism, but with the isotope  
effect for hydroxylation by PheH being masked by tautomerization of an  
dienone intermediate to tyrosine.  
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2004:829478 CAPLUS  
DN 143:50123  
TI Coincidental emission of molecular ions from keV carbon cluster impacts  
AU Locklear, J. E.; Verkhoturov, S. V.; Schweikert, E. A.  
CS Department of Chemistry, Texas A&M University, College Station, TX,  
77842-3012, USA  
SO Int. J. Mass Spectrom. (2004), 238(1), 59-64  
CODEN: IMSPF8; ISSN: 1387-3806  
PB Elsevier B.V.  
DT Journal  
LA English  
AB Exptl. data are reported for the emission of 1 and 2 phenylalanine (Ph)  
mol. ions per impact at 10-21 keV impacts of coronene (C<sub>24</sub>H<sub>12</sub>), C<sub>60</sub>, and

gramicidin S (C60N12O10H92) projectiles as a function of projectile mass, energy, and geometry. Secondary ion mass spectrometry (SIMS) expts. were conducted using event-by-event bombardment and detection. With this method, individual projectile impacts and the resulting secondary ions are recognized as singular events resolved in time and space. The target surface was an equimolar mixture of phenylalanine (PhH, C9H11NO2) and deuterated phenylalanine (PhD, C9H3D8NO2). This allowed for the detection of 2 coemitted [M-H]- phenylalanine ions in a dual time-of-flight instrument. In contrast to the linear dependence yield of Ph vs. energy for single Ph ion emission, the yield for 2 Ph ion emission vs. energy is nonlinear within the exptl. energy range. For the coemission of 2 Ph ions, C60 is more efficient than coronene at equal velocities.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:84896 CAPLUS

DN 140:259439

TI Simultaneous Ejection of Two Molecular Ions from keV Gold Atomic and Polyatomic Projectile Impacts

AU Rickman, R. D.; Verkhoturov, S. V.; Parilis, E. S.; Schweikert, E. A.

CS Department of Chemistry, Texas A&M University, College Station, TX, 77842-3012, USA

SO Physical Review Letters (2004), 92(4), 047601/1-047601/4

CODEN: PRLTAO; ISSN: 0031-9007

PB American Physical Society

DT Journal

LA English

AB We present the first exptl. data on the simultaneous ejection of two mol. ions from the impact of Aun+ ( $1 \leq n \leq 4$ ) with energies ranging between 17 and 56 keV. The yields from single phenylalanine (Ph) emission, coemission of two Ph ions, and emission of the Ph dimer were measured. Large increases (1 to 2 orders of magnitude) in coemitted ion yields were observed with increasing projectile energy and complexity. Correlation coeffs. were calculated for the coemission of two Ph ions; their behavior suggests differences in emission pathways for bombardment by atomic and polyat. projectiles.

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:37331 CAPLUS

DN 137:279427

TI Stereocontrolled synthesis of deuterated phenylalanine derivatives through manipulation of an N-phthaloyl protecting group for the recall of stereochemistry. Application in the study of phenylalanine ammonia lyase

AU Easton, Christopher J.; Fryer, Nicholas L.; Kelly, James B.; Kociuba, Katherine

CS Research School of Chemistry, Institute of Advanced Studies, Australian National University, Canberra, ACT 0200, Australia

SO ARKIVOC [online computer file] (2001), 2(7), No pp. given

CODEN: AKVCFI

URL: [http://www.arkat-usa.org/ARKIVOC/JOURNAL\\_CONTENT/manuscripts/2001/DC-245BP%20as%20published%20mainmanuscript.pdf](http://www.arkat-usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2001/DC-245BP%20as%20published%20mainmanuscript.pdf)

PB ARKAT Foundation

DT Journal; (online computer file)

LA English

OS CASREACT 137:279427

AB The enantiomers of [2-2H1]phenylalanine and all four stereoisomers of [2,3-2H2]phenylalanine have been prepared from (S)-phenylalanine through the introduction of a chiral center onto an N-phthaloyl protecting group for the recall of stereochem. Studies of the interaction of these labeled phenylalanines with (S)-phenylalanine ammonia lyase show that both the C-2

and C-3 hydrogens of the product trans-cinnamate undergo exchange with solvent in the presence of the enzyme. The mechanistic implications of this observation are discussed.

RE.CNT 24      THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5    ANSWER 5 OF 48    CAPLUS    COPYRIGHT 2007 ACS on STN  
AN    2000:135358    CAPLUS  
DN    132:306166  
TI    Intense exercise stimulates albumin synthesis in the upright posture  
AU    Nagashima, Kei; Cline, Gary W.; Mack, Gary W.; Shulman, Gerald I.; Nadel, Ethan R.  
CS    John B. Pierce Laboratory and Departments of Cellular and Molecular Physiology, Epidemiology, and Public Health and Internal Medicine, Yale University School of Medicine, New Haven, CT, 06519, USA  
SO    Journal of Applied Physiology (2000), 88(1), 41-46  
      CODEN: JAPHEV; ISSN: 8750-7587  
PB    American Physiological Society  
DT    Journal  
LA    English  
AB    We tested the hypothesis that an elevation in albumin synthetic rate contributes to increased plasma albumin content during exercise-induced hypervolemia. Albumin synthetic rate was measured in seven healthy subjects at 1-5 and 21-22 h after 72 min of intense (85% peak oxygen consumption rate) intermittent exercise and after 5 h recovery in either upright (Up) or supine (Sup) postures. Deuterated phenylalanine (d5-Phe) was administered by a primed-constant infusion method, and fractional synthetic rate (FSR) and absolute synthetic rate (ASR) of albumin were calculated from the enrichment of d5-Phe in plasma albumin, determined by gas chromatog.-mass spectrometry. FSR of albumin in Up increased significantly ( $P < 0.05$ ) from  $4.9 \pm 0.9\%$ /day at control to  $7.3 \pm 0.9\%$ /day at 22 h of recovery. ASR of albumin increased from  $87.9 \pm 17.0$  to  $141.1 \pm 16.6$  mg albumin  $\cdot$  kg body wt $\cdot$ 1.day $\cdot$ 1. In contrast, FSR and ASR of albumin were unchanged in Sup ( $3.9 \pm 0.4$  to  $4.0 \pm 1.4\%$ /day and  $74.2 \pm 8.9$  to  $85.3 \pm 23.9$  mg albumin $\cdot$ kg body wt $\cdot$ 1.day $\cdot$ 1 at control and 22 h of recovery, resp.). Increased albumin synthesis after upright intense exercise contributes to the expansion of greater albumin content and its maintenance. We conclude that stimuli related to posture are critical in modulating the drive for albumin synthesis after intense exercise.

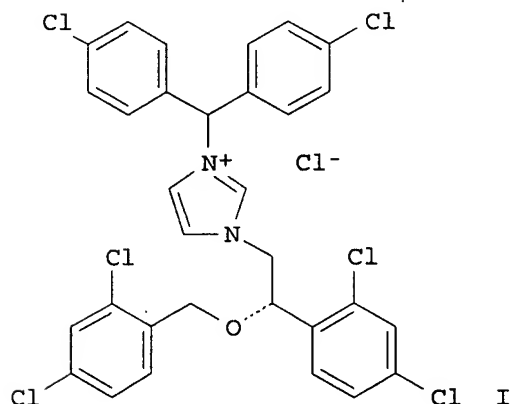
RE.CNT 29      THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5    ANSWER 6 OF 48    CAPLUS    COPYRIGHT 2007 ACS on STN  
AN    1999:654102    CAPLUS  
DN    131:350401  
TI    Determination of deuterated phenylalanine and tyrosine in egg protein by GCQ  
AU    Geypens, Benny; Claus, Dirk; Gorris, Nicole; Evenepoel, Pieter; Luypaerts, Anja; Rutgeerts, Paul; Ghoo, Yvo  
CS    Department of Medicine, Division of Gastroenterology and Gastrointestinal Research Centre, University Hospital Leuven, Louvain, B-3000, Belg.  
SO    Journal of High Resolution Chromatography (1999), 22(8), 465-468  
      CODEN: JHRCE7; ISSN: 0935-6304  
PB    Wiley-VCH Verlag GmbH  
DT    Journal  
LA    English  
AB    In order to study protein digestibility by means of noninvasive tracer techniques (stable isotopes), a representative oral tracer, i.e. a stable isotope labeled protein, is needed. Therefore, egg white containing L-[ring-2H5]phenylalanine and L-[ring-2H4]tyrosine was prepared. The aim of this study was to measure the isotopic enrichment of the labeled amino acids in the egg white. The use of a standard GC-MS, based on ion trap technol. was found to be a reliable technique. The enrichment of L-[ring-2H5]phenylalanine and L-[ring-2H4]tyrosine, expressed in Molar

Percent (MP) amounted to 23.2 MP and 2.8 MP resp.  
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1999:2880 CAPLUS  
DN 130:179199  
TI Stereospecific labeling at  $\alpha$ -position of phenylalanine and  
phenylglycine with amino acid racemase  
AU Lim, Young-Hee; Yoshimura, Tohru; Soda, Kenji; Esaki, Nobuyoshi  
CS Institute for Chemical Research, Kyoto University, Kyoto-Fu, 611-0011,  
Japan  
SO Journal of Fermentation and Bioengineering (1998), 86(4), 400-402  
CODEN: JFBIEX; ISSN: 0922-338X  
PB Society for Fermentation and Bioengineering, Japan  
DT Journal  
LA English  
OS CASREACT 130:179199  
AB Amino acid racemase with low substrate specificity (EC 5.1.1.10) purified  
from *Pseudomonas putida* ATCC17642 catalyzes the racemization of various  
amino acids but not that of aromatic and acidic amino acids. However,  
phenylalanine and phenylglycine underwent  $\alpha$ -hydrogen exchange with  
deuterium from the solvent when incubated with the racemase in deuterium  
oxide. Each enantiomer of both  $\alpha$ -deuterated  
phenylalanine and phenylglycine was produced stereospecifically  
with retention of the C2 configuration. This  $\alpha$ -hydrogen exchange  
reaction is applicable to the production of  $\alpha$ -deuterated  
phenylalanine and phenylglycine.  
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1997:97684 CAPLUS  
DN 126:212091  
TI Synthesis and analysis of the enantiomers of calmidazolium, and a  $^1\text{H}$  NMR  
demonstration of a chiral interaction with calmodulin  
AU Edwards, Andrew J.; Sweeney, Patricia J.; Reid, David G.; Walker, John M.;  
Elshourbagy, Nabil; Egwuagu, Charles E.; Young, James F.; Patton, Curtis  
L.  
CS SmithKline Beecham Pharm., Welwyn, UK  
SO Chirality (1996), 8(8), 545-550  
CODEN: CHRLEP; ISSN: 0899-0042  
PB Wiley-Liss  
DT Journal  
LA English  
GI



AB Calmidazolium [R24571, 1-[bis(4-chlorophenyl)methyl]-3-[2-(2,4-dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl]-1H-imidazolium chloride] is a potent calmodulin inhibitor. In this report, the preparation and properties of enantiomers of calmidazolium were described. For example, (+)-(S)-calmidazolium chloride (I) was prepared. Overlap between ligand and protein resonances in the aromatic region of the <sup>1</sup>H NMR spectrum of the calmidazolium-calmodulin complexes was obviated by preparation of the protein with all of its nine phenylalanine rings deuterated (Phe-d<sub>5</sub> calmodulin). This was accomplished by the over-expression of calmodulin derived from *Trypanosoma brucei rhodesiense* in *E. coli* in a medium supplemented with ring-deuterated phenylalanine. The kinetics of binding of each enantiomer were slow on the <sup>1</sup>H NMR time scale as judged by the behavior of the H<sub>2</sub> resonance of Histidine-107, which is clearly visible under the sample conditions used. The aromatic spectral regions of the protein-bound (+) and (-) enantiomers contrasted strikingly, reflecting differences in bound environment and/or conformation.

L5 ANSWER 9 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:811899 CAPLUS

DN 124:30298

TI GC/MS analysis of [2H<sub>5</sub>]phenylalanine at very low enrichment: measurement of protein synthesis in health and disease

AU Slater, Christine; Preston, Tom; McMillan, Donald C.; Falconer, J. Stuart; Fearon, Kenneth C. H.

CS Isotope Biochemistry Laboratory, Scottish Universities Research and Reactor Centre, Glasgow, G75 0QF, UK

SO Journal of Mass Spectrometry (1995), 30(9), 1325-32  
CODEN: JMSPFJ; ISSN: 1076-5174

PB Wiley

DT Journal

LA English

AB A gas chromatog./mass spectrometric (GC/MS) method has been developed for the precise and accurate anal. of high enrichment (1-10 mol. % excess) and very low enrichment (0.005-0.12 mol. % excess) 2H<sub>5</sub>-labeled phenylalanine. Tracer enrichment in free phenylalanine was measured by GC/electron impact MS anal. of the tert-butyldimethylsilyl (TBDMS) derivative. The measurement of very low tracer enrichment, typical of that found in protein hydrolyzates, was accomplished by careful control of sample yield during preparation and anal. of the TBDMS derivative of purified β-phenylethylamine, produced by enzymic decarboxylation and solvent extraction. The new method was illustrated by measurement of albumin synthesis in healthy patients using a rapid protocol which showed good patient acceptability and was straightforward to manage in the clin. setting. The mean (SEM) albumin fractional synthetic rate was 9.54% (0.81%) per day, in agreement with previous studies that used more complex clin. protocols and anal. procedures. Use of the same derivative for anal. of amino acid precursor and protein samples facilitated consecutive anal. on the same instrument without interruption, permitting rapid feedback of results to the clinician and the possibility of using the method in intervention studies. The method should prove useful in the study of the synthetic rate of other proteins and mixed tissue protein, which will help understanding and management of protein metabolism in health and disease. The possibility of extending the use of multiple-atom tracers combined with GC/MS anal. to other substrate metabolism studies was identified.

L5 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:578974 CAPLUS

DN 123:78236

TI Mechanism of metal-independent hydroxylation by *Chromobacterium violaceum* phenylalanine hydroxylase

AU Carr, Robert T.; Balasubramanian, Shankar; Hawkins, Paul C. D.; Benkovic, Stephen J.

CS Department of Chemistry, Pennsylvania State University, University Park,

PA, 16802, USA  
SO Biochemistry (1995), 34(22), 7525-32  
CODEN: BICHAW; ISSN: 0006-2960  
PB American Chemical Society  
DT Journal  
LA English  
AB Phenylalanine hydroxylase (PAH) converts phenylalanine to tyrosine utilizing a tetrahydrobiopterin cofactor. Several key mechanistic questions have yet to be resolved, specifically the identity of the hydroxylating species and the role of the nonheme Fe which is present in all of the mammalian PAHs. Recently, the authors demonstrated that a bacterial PAH from *C. violaceum* (CVPAH) does not require any redox active metal for activity. To identify the function of Fe in the mammalian PAHs, the authors undertook a series of expts. to compare the mechanisms of this metal-independent CVPAH with the Fe-dependent PAH from rat liver (RLPAH). Using [4-2H]phenylalanine as a substrate gave a kinetic isotope effect on hydroxylation of unity for CVPAH which was in agreement with previous values reported for RLPAH. The [4-2H]phenylalanine underwent an NIH shift upon hydroxylation by CVPAH. The extent of 2H retention at the 3-position of the tyrosine product was identical within exptl. error for both RLPAH and CVPAH using [4-2H]phenylalanine and [2,3,5,6-2H]phenylalanine as substrates. This suggests that PAH from either source probably does not directly mediate the NIH shift mechanism. No uncoupled pterin turnover was observed for CVPAH with either L-tyrosine or p-chloro-L-phenylalanine as substrate or tetrahydropterin as cofactor, each of which causes uncoupled turnover with RLPAH. CVPAH readily accepts 4-methylphenylalanine as a substrate giving 4-(hydroxymethyl)phenylalanine as the major product and 3-methyltyrosine as the only other minor product. The ratio of alkyl to aromatic hydroxylation was very close to a ratio previously obtained for this analog and 2 deuterated analogs. This suggests that both RLPAH and CVPAH utilize a very similar oxygenating intermediate. The authors also demonstrated that both metal-free and Fe-dependent enzymes hydroxylated cyclohexylalanine in a stereoselective manner.

L5 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1995:469834 CAPLUS  
DN 122:260360  
TI Comparison of [5,5,5-2H3]leucine and [ring-2H5]phenylalanine tracers for the measurement of human apolipoprotein B100 kinetics  
AU Maugeais, C.; Ouguerram, K.; Maugeais, P.; Simoneau, C.; Gardette, J.; Magot, T.; Krempf, M.  
CS Lab. Nutrition Humaine, Hopital G. & R. Laennec, Nantes, 44035, Fr.  
SO Journal of Mass Spectrometry (1995), 30(3), 478-84  
CODEN: JMSPFJ; ISSN: 1076-5174  
PB Wiley  
DT Journal  
LA English  
AB Incorporation of amino acids labeled with stable isotopes in apolipoproteins is used to estimate kinetic aspects of lipoprotein metabolism

In

this study two deuterated tracers, [5,5,5-2H3]leucine and [ring-2H5]phenylalanine, were compared. Isolation and acid hydrolysis of apolipoproteins are required for mass spectrometric anal. When apolipoprotein B100 of very-low-d. lipoproteins was prepared with this procedure, a loss of deuterium was observed on deuterated phenylalanine with 10 and 6 M HCl hydrolysis but not with deuterated leucine or when 4 M HCl hydrolysis was used. This study stresses the effect of acid hydrolysis on [ring-2H5]phenylalanine. This tracer must be used with caution in studies of specific protein synthesis.

L5 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1995:273259 CAPLUS  
DN 122:133752  
TI Synthesis of each stereoisomer of [3-2H1]phenylalanine and evaluation of the stereochemical course of the reaction of (R)-phenylalanine with

(S)-phenylalanine ammonia-lyase  
 AU Easton, Christopher J.; Hutton, Craig A.  
 CS Dep. Chem., Univ. Adelaide, SA 5005, Australia  
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and  
 Bio-Organic Chemistry (1994); (24), 3545-8  
 CODEN: JCPRB4; ISSN: 0300-922X  
 PB Royal Society of Chemistry  
 DT Journal  
 LA English  
 OS CASREACT 122:133752  
 AB The four stereoisomers of [3-2H]phenylalanine have been prepared, each as a  
 single enantiomer in ca. 98% diastereoisomeric excess and with ca. 99%  
 deuterium incorporation, by side-chain bromination of phenylalanine  
 derivs., followed by deuteriolysis of each of the diastereoisomeric  
 product bromides with deuterium over 5% palladium-on-carbon. The latter  
 reactions proceeded with retention of configuration. (2R,3S)-[3-  
 2H]phenylalanine reacted with (S)-phenylalanine ammonia-lyase to give  
 [3-2H]-trans-cinnamic acid, with 92% deuterium incorporation, while the  
 (2R,3R)-stereoisomer phenylalanine gave [3-2H]-trans-cinnamic acid with  
 27% deuterium incorporation. These results indicate that reaction of  
 (R)-phenylalanine with the enzyme involves mainly loss of the 3-pro-R  
 hydrogen and ammonia, in an antiperiplanar elimination process analogous  
 to that previously reported for (S)-phenylalanine, while a minor pathway  
 for reaction of (R)-phenylalanine is either isomerization to  
 (S)-phenylalanine, before elimination, or synperiplanar elimination.

L5 ANSWER 13 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1994:552611 CAPLUS  
 DN 121:152611  
 TI Response of protein synthesis in human skeletal muscle to insulin: an  
 investigation with L-[2H5]phenylalanine  
 AU McNurlan, M. A.; Essen, P.; Thorell, A.; Calder, A. G.; Anderson, S. E.;  
 Ljungqvist, O.; Sandgren, A.; Grant, I.; Tjader, I.; et al.  
 CS Rowett Res. Inst., Aberdeen, AB2 9SB, UK  
 SO American Journal of Physiology (1994), 267(1, Pt. 1), E102-E108  
 CODEN: AJPHAP; ISSN: 0002-9513  
 DT Journal  
 LA English  
 AB The role of insulin in the regulation of muscle protein synthesis in adult  
 humans has been investigated with i.v. infusion of insulin at levels  
 comparable with those observed after normal feeding. Glucose was also  
 infused to maintain euglycemia. Muscle protein synthesis was measured in  
 six healthy subjects before and during insulin and glucose infusion from  
 the incorporation of L-[2H5]phenylalanine into the protein of vastus  
 lateralis sampled by percutaneous biopsy. L-[2H5]phenylalanine was given  
 as a single injection of a flooding amount (45 mg/kg). The relatively low  
 levels of enrichment of phenylalanine in protein (0.005 atom%) were  
 measured by modified gas chromatog.-mass spectrometry and verified by  
 comparison with incorporation of L-[2,6-3H]phenylalanine. Similarity of  
 enrichment of phenylalanine in tissue-free and plasma pools (flooding) and  
 linear incorporation over the period of measurement were also verified.  
 The fractional rate of muscle protein synthesis in the group of  
 postabsorptive subjects was 1.65%/day. The rate was unaltered by insulin  
 and glucose infusion, 1.66%/day.

L5 ANSWER 14 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1994:164847 CAPLUS  
 DN 120:164847  
 TI Kinetic Isotope Effects on Hydroxylation of Ring-Deuterated  
 Phenylalanines by Tyrosine Hydroxylase Provide Evidence against  
 Partitioning of an Arene Oxide Intermediate  
 AU Fitzpatrick, Paul F.  
 CS Department of Chemistry and Biochemistry and Biophysics, Texas A and M  
 University, College Station, TX, 77843-2128, USA  
 SO Journal of the American Chemical Society (1994), 116(3), 1133-4

CODEN: JACSAT; ISSN: 0002-7863

DT Journal  
LA English

AB When Phe is used as a substrate for rat tyrosine hydroxylase, both Tyr and 3-hydroxyphenylalanine are formed in a 26:1 ratio. To test whether this is due to partitioning of an arene oxide intermediate, ring-deuterated phenylalanines were characterized as substrates for the enzyme. With 4-deuterophenylalanine, an isotope effect of 1.2 is found on the rate of Tyr formation, but no effect is seen on the rate of 3-hydroxyphenylalanine formation. With 3,5-dideuterophenylalanine, an isotope effect of about 1.7 is found on the rate of 3-hydroxyphenylalanine formation, but the rate of Tyr formation is unaffected. Results with perdeuterated substrate are consistent with the independence of the effects of substitution in the ring. These results are not predicted for the partitioning of an obligatory arene oxide mechanism.

L5 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1993:406249 CAPLUS  
DN 119:6249

TI In vivo determination of phenylalanine hydroxylase activity in cirrhotic patients with 2H-phenylalanine

AU Dai, Tengchang; Xia, Zongqin; Zhang, Jianhua; Hu, Yaer; Lu, Hanming; Li, Xuanhai; Peng, Xiaowei; Shi, Qianghua; Xu, Xinrong; et al.

CS Dep. Exp. Nucl. Med., Shanghai 2nd Med. Univ., Shanghai, Peop. Rep. China  
SO Tongweisu (1992), 5(1), 31-5

CODEN: TONGEM; ISSN: 1000-7512

DT Journal  
LA Chinese

AB The phenylalanine hydroxylase activities of 23 cirrhotic patients (8 compensated and 15 decompensated) and 8 normal adults were measured with a deuterated phenylalanine (PMe)-loading test. After a single i.v. injection of 10 mg/kg labeled L-Phe or 20 mg/kg labeled DL-Phe, the abundances of plasma Phe and Tyr were analyzed with GC-MS. The activities of Phe hydroxylase were estimated by the slope of Tyr abundance curve, the slope of Tyr/Phe abundance ratio curve, the area under Tyr abundance curve, and the area under Tye/Phe abundance ratio curve. The results revealed that the activity of Phe hydroxylase was impaired in cirrhotic patients and the impairment was more severe in decompensated than in compensated cirrhosis.

L5 ANSWER 16 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1992:527661 CAPLUS  
DN 117:127661

TI The determination of low d5-phenylalanine enrichment (0.002-0.09 atom percent excess), after conversion to phenylethylamine, in relation to protein turnover studies by gas chromatography/electron ionization mass spectrometry

AU Calder, A. G.; Anderson, S. E.; Grant, I.; McNurlan, M. A.; Garlick, P. J.

CS Rowett Res. Inst., Bucksburn, AB2 9SB, UK

SO Rapid Communications in Mass Spectrometry (1992), 6(7), 421-4

CODEN: RCMSEF; ISSN: 0951-4198

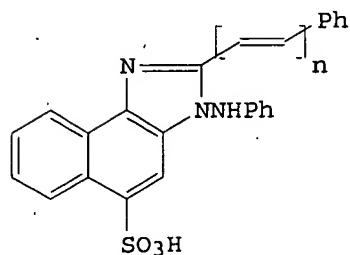
DT Journal  
LA English

AB A gas chromatog./mass spectrometry (GC/MS) method for measuring very low levels of enrichment of d5-phenylalanine (0.002-0.09 atom percent excess) is described. This method makes it possible to determine the enrichment of amino acid incorporated into tissue protein during studies of protein synthesis in man. Phenylalanine is enzymically converted to phenylethylamine and the d5-enrichment is measured in the heptafluorobutyryl derivative by selective-ion recording under electron ionization conditions. The coeffs. of variation for muscle-protein hydrolyzate samples enriched with d5-phenylalanine at the 0.005 and 0.05 atom percent excess levels were 6.0 and 1.2%, resp. This precision at low enrichment and the small amount of protein needed (about 1 mg) provide real

advantages for clin. studies of tissue protein synthesis. Moreover, in contrast to the conventional approach which uses GC/MS for plasma amino acids (typically 2-20 atom percent excess) but gas isotope-ratio mass spectrometry for protein-bound amino acids, the enrichment of both plasma-free and protein-bound d5-phenylalanine can be measured with a single instrument.

L5 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1991:425784 CAPLUS  
 DN 115:25784  
 TI Formation of toluene by microorganisms from anoxic freshwater sediments  
 AU Juettner, Friedrich  
 CS Abt. Oekophysiologie, Max-Planck-Inst. Limnol., Ploen, W-2320, Germany  
 SO Fresenius' Journal of Analytical Chemistry (1991), 339(10), 785-7  
 CODEN: FJACES; ISSN: 0937-0633  
 DT Journal  
 LA English  
 AB In artificial anoxic lakewater that had been inoculated with anoxic lake sediment, toluene was liberated by microorganisms and accumulated in the water. Phenylalanine, phenyllactate and phenylpyruvate proved to be effective precursors. Media supplemented with phenylacetate developed toluene even in a shorter period of time than the other three compds. 2-Phenylethanol, phenylacetaldehyde, and phenylacetic acid Et ester only weakly supported the formation of toluene. The effectiveness of benzaldehyde was very low, and cinnamate did not at all support the formation of toluene. The transformation of phenylalanine to toluene was complete and resulted in the formation of stoichiometric amts. Labeling expts. with deuterated phenylalanine showed no loss of label in the toluene mol. and no dilution by unlabeled toluene. The expts. support the view that phenylalanine that has been liberated from proteinaceous matter by hydrolysis is degraded in anoxic hypolimnia of lakes and anoxic sediments of rivers only to the stage of toluene. This reaction is responsible for the accumulation of toluene in these environments.

L5 ANSWER 18 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1990:52933 CAPLUS  
 DN 112:52933  
 TI Conformation-activity relationship of sweet molecules. Comparison of aspartame and naphthimidazolesulfonic acids  
 AU Castiglione-Morelli, M. A.; Lelj, F.; Naider, F.; Tallon, M.; Tancredi, T.; Temussi, P. A.  
 CS Dip. Chim., Univ. Basilicata, Potenza, Italy  
 SO Journal of Medicinal Chemistry (1990), 33(2), 514-20  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 GI



I, n=1

II, n=0

AB The shape of the active site of the receptor for sweet mols. was previously defined on the basis of a combination of both rigid (saccharins) and flexible (aspartame) molds. The sweetness receptor is

refined by using the shapes of 3-anilino-2-styryl-3H-naphth[1,2-d]imidazolesulfonate (I) (sweet) and 3-anilino-2-phenyl-3H-naphth[1,2-d]imidazolesulfonate (II) (tasteless), 2 large and almost completely rigid tastants. The min.-energy conformations of the flexible portions of these tastants were determined by using a detailed conformational anal. based on ab initio calcns. The refined receptor site is still consistent with all previously examined sweet mols. To assay unequivocally the prochiral  $\beta$ -CH<sub>2</sub> protons of the phenylalanine moiety of aspartame,  $\alpha$ -L-Asp-L-2S,3S-2H<sub>2</sub>)PheOMe was synthesized and examined by using 500-MHz 1H NMR spectroscopy. The min.-energy conformation for aspartame in water, [2H<sub>6</sub>]DMSO, and CDCl<sub>3</sub> (as a crown ether complex) was different from that originally proposed (FIIDII instead of FIDII, according to a notation referring to the side chains). Although this conformation is not directly consistent with the shape of the sweet receptor, the interconversion of FIIDII to FIDII required only 1 kcal/mol. Furthermore a 120-ps mol. dynamics simulation in vacuo confirmed the high flexibility of aspartame and the accessibility of the FIDII conformer whose topol. is fully consistent with the present model.

L5 ANSWER 19 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1989:452787 CAPLUS

DN 111:52787

TI NMR line broadening study of hydrophobic peptides interaction with phospholipid bilayers

AU Khabarova, E. I.; Dubovskii, P. V.; Vasilenko, I. A.; Zvonkova, E. N.; Gusev, D. G.; Ogrel, A. A.

CS M. V. Lomonosov Inst. Fine Chem. Technol., Moscow, USSR

SO Biologicheskoe Membrany (1989), 6(4), 378-85

CODEN: BIMEE9; ISSN: 0233-4755

DT Journal

LA Russian

AB Octadecyl esters of glycine, L-Ala-Gly, L-Phe-L-Ala-Gly, and their 2H-labeled derivs. were synthesized. The prepared peptides were introduced into a phospholipid bilayer, and the modified membrane was studied by wide-line 2H and 31P NMR. The observed behavior of the peptide esters in the bilayer did not seem to depend on the length of the peptide fragment. Addition of octadecyl peptides to egg lecithin with subsequent hydration gave homogeneous mixts. of distinct bilayer structure. Glycine octadecyl ester on dispersion in water in the absence of phospholipid was capable of forming multilamellar aggregates in a wide concentrational range (10<sup>-1</sup>-10<sup>-3</sup>M), whereas H-L-Ala-Gly-OC18H37 and H-L-Phe-L-Ala-Gly-OC18H37 under the same conditions did not give any vesicular structures.

L5 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1988:473499 CAPLUS

DN 109:73499

TI Asymmetric synthesis with boronic esters

AU Matteson, Donald S.

CS Dep. Chem., Washington State Univ., Pullman, WA, 99164-4630, USA

SO Accounts of Chemical Research (1988), 21(8), 294-300

CODEN: ACHRE4; ISSN: 0001-4842

DT Journal; General Review

LA English

AB A review, containing 53 refs., summarizes the enantioselective syntheses of natural products ranging from insect pheromones to L-ribose to chirally deuterated phenylalanine and D-glyceraldehyde utilizing the method of insertion of asym. carbon into an existing boron-carbon bond of boronic esters.

L5 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1988:71583 CAPLUS

DN 108:71583

TI A multiple stable isotope tracer technique for studying the metabolic kinetics of amino acids in hepatic failure

AU Xia, Zongqin; Dai, Tengchang; Zhang, Jianhua; Hu, Yaer; Yu, Bingyao; Xu,

Xingrong; Huang, Guanlu; Shen, Gengrong; Zhou, Yaqiu; et al.  
CS Shanghai 2nd Med. Univ., Shanghai, Peop. Rep. China  
SO Hejishu (1987), 10(8), 45-53  
CODEN: NUTEDL; ISSN: 0253-3219  
DT Journal  
LA English  
AB To study the mechanism of the imbalance of amino acid metabolism during hepatic failure, a stable isotope tracer method for observing simultaneously the metabolic kinetics of several amino acids has been established. L-[15N]alanine, [2,3-D3]leucine and [2,3-D3]phenylalanine were chosen as nonessential, branched chain and aromatic amino acids. A single i.v. injection of 40 mg [15]alanine, 20 mg deuterated leucine, and 20 mg deuterated phenylalanine was given to each human subject. Blood samples were taken just before and at different times ( $\leq 60$  min) after the injection. Total free amino acids were isolated from the plasma with a small Dowex 50 + 8 column and converted to trifluoroacetyl derivs. Their abundances were then analyzed with a GC-mass spectrometry (MS) system and typical double exponential time course curves were found for all 3 labeled amino acids. A 2-pool model was designed and applied for compartmental anal. Significant changes were found in the kinetic parameters of phenylalanine and leucine in patients with fulminant hepatitis or hepatic cirrhosis. The half-lives of both phenylalanine pools were longer and the pool sizes were larger than normal subjects, whereas the half-lives and pool sizes of leucine changed in the opposite direction. No marked change was found in alanine. The significance of intracellular imbalance of phenylalanine and leucine metabolism was discussed. It is evident that the combination of GC-MS technique and multiple-tracers labeled with stable isotopes is of great potential for similar purposes.

L5 ANSWER 22 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1987:193409 CAPLUS  
DN 106:193409  
TI The contributions of phenylethanolamine and p-octopamine metabolism towards the urinary excretion of mandelic acid, p-hydroxymandelic acid, phenylglycol and p-hydroxyphenylglycol in rats  
AU Karoum, F.; Chuang, L. W.  
CS Saint Elizabeths Hosp., Natl. Inst. Ment. Health, Washington, DC, 20032, USA  
SO Biogenic Amines (1987), 4(1), 1-7  
CODEN: BIAME7; ISSN: 0168-8561  
DT Journal  
LA English  
AB Mass fragmentog. was employed in the assay of mandelic acid (MA), phenylglycol (PG), p-hydroxymandelic acid (PHMA), and p-hydroxyphenylglycol (PHPG) in rat urine after a number of pharmacol. manipulations. The purpose of this study was primarily to determine the origins of these metabolites in urine. Chronic treatments with neomycin, MAO inhibitors, and carbidopa failed to markedly reduce the excretions of MA or PHMA, suggesting that these purported acidic metabolites of phenylethanolamine and p-octopamine do not primarily originate from the gut or from their expected precursor monoamines. The MAO inhibitors, deprenyl and clorgyline significantly reduced the excretion of PG and PHPG, indicating that the excretion of these neutral metabolites better reflect the metabolism of their precursor monoamines than do the acidic metabolites. The administration of phenylethanolamine and p-octopamine led to a marked increase in both the acidic and neutral metabolites. However, the ratios of the acidic to the neutral metabolites observed after these treatments were opposite to those found in normal urine. The ratio of MA to PG observed after phenylethanolamine administration was .apprx.8:1 whereas that of p-octopamine metabolites was .apprx.1:6. These ratios are almost the reverse of the normal ratios. It is, therefore, concluded that the metabolic processes normally responsible for the formation of MA and PHMA may not be identical to those which mediate the metabolism of exogenously administered phenylethanolamine and p-octopamine. Efforts to study these

alternative pathways employing deuterated phenylalanine and tyrosine administrations to rats pretreated with carbidopa suggest that MA and PHMA are formed from pathways involving transamination of phenylalanine and p-tyrosine, resp. The possibility was then tested to determine how can  $\beta$ -hydroxylated acidic metabolites be formed from these amino acids. The effects of administering phenylserine, p-hydroxyphenylserine, phenylpyruvic acid, and p-hydroxyphenylpyruvic acid were evaluated on MA and PHMA excretions. Phenylpyruvic acid and p-hydroxyphenylpyruvic acid are transaminated products of phenylalanine and p-tyrosine. The results suggested minor roles of phenylserine and p-hydroxyphenylserine. p-Hydroxyphenylpyruvic acid administration markedly increased PHMA excretion, suggesting that most urine PHMA probably originates from this compound

- L5 ANSWER 23 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1986:622085 CAPLUS  
 DN 105:222085  
 TI The NIH-shift in the in vivo hydroxylation of ring-deuterated L-phenylalanine in man  
 AU Lehmann, Wolf D.; Heinrich, Hellmuth C.  
 CS Inst. Physiol. Chem., Univ. Hosp. Eppendorf, Hamburg, D-2000/20, Fed. Rep. Ger.  
 SO Archives of Biochemistry and Biophysics (1986), 250(1), 180-5  
 CODEN: ABBIA4; ISSN: 0003-9861  
 DT Journal  
 LA English  
 AB Oral loading with L-[ring-2H5]phenylalanine was performed a a dose of 25 mg/kg for detection of heterozygotes for classic phenylketonuria. By using 3 differently labeled batches of ring-deuterated L-phenylalanine, quant. anal. of 2H-labeled L-phenylalanine and L-tyrosine in plasma revealed different label distributions. Three different reaction mechanisms for the 4-hydroxylation of L-phenylalanine to L-tyrosine were used as the basis for model calcns. of the transformation of the L-phenylalanine label distribution into that of L-tyrosine. The best agreement between observed and calculated distributions was found for the mechanism involving a migration of the 4-substituent into the 3- or 5-position (NIH-shift), followed by a random loss of the 4-/3- or the 4-/5-substituent from this intermediate structure.
- L5 ANSWER 24 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1986:587064 CAPLUS  
 DN 105:187064  
 TI Sensitive determination of deuterated and non-deuterated phenylalanine and tyrosine in human plasma by combined capillary gas chromatography-negative ion chemical ionization mass spectrometry  
 AU Hayashi, Tokishi; Minatogawa, Yukiko; Kamada, Satoru; Shimamura, Michio; Naruse, Hiroshi; Iida, Yoshio  
 CS Natl. Cent. Nerv., Ment. Musc. Disord., Kodaira, 187, Japan  
 SO Journal of Chromatography (1986), 380(2), 239-45  
 CODEN: JOCRAM; ISSN: 0021-9673  
 DT Journal  
 LA English  
 AB A combined capillary gas chromatog.-neg.-ion chemical-ionization mass spectrometric method for the determination of deuterated and nondeuterated phenylalanine and tyrosine in blood plasma was developed. Phenylalanine and tyrosine were converted to pentafluorobenzyl-trifluoroacetyl (PFB-TFA) and PFB-TFA-trimethylsilyl (TMS) derivs., resp., after prepurifn. with a Bio-Rad AG 50W-X2 cation-exchange column. These derivs. showed good gas chromatog. separation properties and provided intense (M-PFB)- ions. These ions were ideal for the specific and sensitive determination of deuterated and nondeuterated phenylalanine and tyrosine by selected ion monitoring assay. [2,2',3,3,3',4',5',6'-2H8]L-Phenylalanine and [2,2',3,3,3',5',6'-2H7]L-tyrosine were used as internal stds. This method was used to determine the plasma levels of deuterated and nondeuterated phenylalanine and tyrosine, after oral administration of [2',3',4',5',6'-2H5]L-phenylalanine to a

healthy person.

- L5 ANSWER 25 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1986:65352 CAPLUS  
DN 104:65352  
TI Sensitive determination of tyrosine metabolites, p-hydroxyphenylacetic acid, 4-hydroxy-3-methoxyphenylacetic acid and 4-hydroxy-3-methoxymandelic acid, by gas chromatography-negative-ion chemical-ionization mass spectrometry. Application to a stable isotope-labelled tracer experiment to investigate their metabolism in man  
AU Shimamura, Michio; Kamada, Satoru; Hayashi, Tokishi; Naruse, Hiroshi; Iida, Yoshio  
CS Natl. Cent. Nervous, Mental Muscular Disord., Tokyo, 187, Japan  
SO Journal of Chromatography (1986), 374(1), 17-26  
CODEN: JOCRAM; ISSN: 0021-9673  
DT Journal  
LA English  
AB A method was established for studying the dynamic metabolism of tyrosine to its metabolites in humans using a deuterium-labeled amino acid. Phenylalanine-d5 was administered orally to human subjects (5 mg/kg), and the levels of p-hydroxyphenylacetic acid-d4, 4-hydroxy-3-methoxyphenylacetic acid-d3, and 4-hydroxy-3-methoxymandelic acid-d3 excreted into urine every h were determined by gas chromatog.-neg.-ion chemical-ionization mass spectrometry. This method was also applied to patients with depression and it was possible to detect a slight alteration in the excretion of some compds. compared with the control.
- L5 ANSWER 26 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1985:25015 CAPLUS  
DN 102:25015  
TI Facile synthesis of (2R,3R)-phenylalanine-2,3-d2 and NMR study on deuterated gramicidin S  
AU Tanimura, Kenjiro; Kato, Tetsuo; Waki, Michinori; Lee, Sannamu; Kodera, Yasushi; Izumiya, Nobuo  
CS Fac. Sci., Kyushu Univ., Fukuoka, 812, Japan  
SO Bulletin of the Chemical Society of Japan (1984), 57(8), 2193-7  
CODEN: BCSJAS; ISSN: 0009-2673  
DT Journal  
LA English  
AB (2R,3R)-Phenylalanine-2,3-d2 (D-Phe-2,3-d2) was prepared by the deuteration of cyclo[(Z)- $\Delta$ Phe-D-Ala] by 2H2 over Pd/C followed by acid hydrolysis of the resulting deuterated cyclic dipeptide. D-Phe-2,3-d2 was used in the synthesis of [D-Phe-2,3-d24,4']-gramicidin S (I) using conventional methods. The NMR of I in (CD3)2SO provided evidence for assignments of D-Phe  $\beta$ -protons in gramicidin S based on the proposal that the predominant rotamer of D-Phe aromatic side chains is the one with  $\kappa_1 = 180^\circ$ .
- L5 ANSWER 27 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1984:589427 CAPLUS  
DN 101:189427  
TI Distances of tyrosine residues from a spin-label hapten in the combining site of a specific monoclonal antibody  
AU Anglister, Jacob; Frey, Tom; McConnell, Harden M.  
CS Stauffer Lab. Phys. Chem., Stanford Univ., Stanford, CA, 94305, USA  
SO Biochemistry (1984), 23(22), 5372-5  
CODEN: BICHAW; ISSN: 0006-2960  
DT Journal  
LA English  
AB The NMR spectra of an Fab fragment of a monoclonal antibody specifically directed against a nitroxide spin-labeled hapten have been recorded at different concns. of the hapten. The hybridoma producing this antibody was grown on deuterated phenylalanine, tryptophan, and 3,5-dideuteriotyrosine or 2,6-dideuteriotyrosine. Difference spectra, without hapten minus with hapten, were calculated for each concentration of hapten.

The difference spectra reveal 5 well-resolved singlet proton resonance signals from tyrosine deuterated in the 3,5-positions (H 2,6 Tyr) and 9 from tyrosine deuterated in the 2,6-positions (H 3,5 Tyr). The measured intensities of these signals as a function of combining site occupation have been interpreted in terms of a theory involving intrinsic line widths (T2), the hapten off-rate (k), and distances to the paramagnetic center. Good agreement with theory is found for all of the isolated proton signals. The best estimate of k (the off-rate of hapten dissociation) is 350

s-1;

distances in the range 13 to <9 Å are calculated. Extension of this anal. to other amino acids is discussed.

L5 ANSWER 28 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1984:571693 CAPLUS

DN 101:171693

TI Synthesis of (2R,3R)-phenylalanine-2,3-d2 and its application to gramicidin S conformation study

AU Tanimura, Kenjiro; Kato, Tetsuo; Lee, Sannamu; Waki, Michinori; Koder, Yasushi; Izumiya, Nobuo

CS Fac. Sci., Kyushu Univ., Fukuoka, 812, Japan

SO Peptide Chemistry (1984), Volume Date 1983, 21st., 81-4

CODEN: PECHDP; ISSN: 0388-3698

DT Journal

LA English

AB The title deuterated amino acid (H-D-Phe\*-OH) was prepared from cyclo(Gly-D-Ala) (I) via a stereoselective deuteration. Thus, I was converted to cyclo(ΔPhe-D-Ala), which was deuterated with D2 over Pd/C to give 97% cyclo(D-Phe\*-D-Ala) (II) with 98.8% chiral induction. II was hydrolyzed by 6N HCl to give 80% H-D-Phe\*-OH. H-Phe\*-OH was used in the synthesis of deuterated gramicidin S (GS) cyclo(Val-Orn-Leu-D-Phe\*-Pro)2 (III) by conventional solution methods. The NMR of III confirmed κ1 = 180° for the conformation of the D-Phe side chain in GS.

L5 ANSWER 29 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1984:68704 CAPLUS

DN 100:68704

TI Facile synthesis of (2R,3R)-phenylalanine-2,3-d2 and its application to conformational analysis of gramicidin S

AU Tanimura, Kenjiro; Kato, Tetsuo; Waki, Michinori; Izumiya, Nobuo

CS Fac. Sci., Kyushu Univ., Fukuoka, 812, Japan

SO Tetrahedron Letters (1983), 24(35), 3737-40

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

AB (2R,3R)-Phenylalanine-,3-d2(I) was prepared in good yield by catalytic reduction

of cyclo(2,3-dehydrophenylalanyl-D-alanyl) under an atmospheric of 2H2 followed by hydrolysis. I was used to synthesize gramicidin S containing the deuterated D-phenylalanine and the 1H NMR of the product was used in conformation anal. studies.

L5 ANSWER 30 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1982:212975 CAPLUS

DN 96:212975

TI The use of deuterated phenylalanine for the in vivo assay of phenylalanine hydroxylase activity in children

AU Matalon, R.; Matthews, D. E.; Michals, K.; Bier, D.

CS Dep. Pediatr., Univ. Illinois, Chicago, IL, 60612, USA

SO Journal of Inherited Metabolic Disease (1982), 5(1), 17-19

CODEN: JIMDDP; ISSN: 0141-8955

DT Journal

LA English

AB Children, 5 with phenylketonuria (PKU), 5 with hyperphenylalaninemia, and 5 phenotypically normal but at risk of being carriers of PKU, were given [ring-2H5]phenylalanine orally in amts. ranging 10-75 mg/kg. Plasma was

assayed for [2H5]phenylalanine and [2H4]tyrosine at hourly intervals, the amino acids being measured as the N-acetyl, Pr esters by gas chromatog.-mass spectroscopy. The results obtained were calculated as the log of the ratio [2H5]phenylalanine:[2H4]tyrosine in the plasma. The 5 patients with PKU had ratios of infinity because no [2H4]tyrosine was measured in their plasma during the exptl. period. The patients with hyperphenylalaninemia had log ratios >2.00 throughout the assay period. Among the 5 normal children 3 are considered to be carriers for PKU as the logarithms of the [2H5]phenylalanine:[2H4]tyrosine ratios were 1.77, 1.73, and 1.33, and remained >1.00 during the assay period. The other children had log ratios of 1.16 and 1.00 at the 1st h which dropped to <1.00 subsequently, suggesting normal activity of phenylalanine hydroxylase.

L5 ANSWER 31 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1982:80145 CAPLUS

DN 96:80145

TI The conformational properties of somatostatin. IV. The conformers contributing to the conformational equilibrium of somatostatin in aqueous solution as found by semi-empirical energy calculations and high-resolution NMR experiments

AU Knappenberg, M.; Michel, A.; Scarso, A.; Brison, J.; Zanen, J.; Hallenga, K.; Deschrijver, P.; Van Binst, G.

CS Lab. Chim. Biol., Univ. Etat Mons, Mons, 7000, Belg.

SO Biochimica et Biophysica Acta, Protein Structure and Molecular Enzymology (1982), 700(2), 229-46

CODEN: BBAEDZ; ISSN: 0167-4838

DT Journal

LA English

AB The results of conformational study by <sup>1</sup>H and <sup>13</sup>C high-resolution NMR at 270 and 500 MHz on the cyclic somatostatin [38916-34-6] were compared with a series of conformers generated by semiempirical energy calcns. The use of specifically deuterated phenylalanine residues enabled the identification of all but the phenylalanine aromatic resonances in the proton spectra of somatostatin. To minimize the risk of overlooking some low-energy conformations, 4 different strategies were used for the generation of the conformers: 2 based on combinations of conformations of fragments that had been studied before, one on a random procedure, and one of the conformational constraints existing in bicyclic analogs with high biol. activity. The exptl. values of <sup>3</sup>J<sub>NH-CαH</sub> and <sup>3</sup>J<sub>αβ</sub> coupling consts. and the existence of several ring current shifts allowed the selection from the calcns. those families of low-energy conformers that were compatible with the NMR results. The NH temperature coeffs. did not warrant the existence of any stable β or γ turns in the mol., although the region 8-12-somatostatin seems to be the most stable in this respect. In addition there are several upfield shifts: 0.2-0.4 ppm on the lysine9 side-chain, 0.3-0.5 ppm on the phenylalanine6α,β and phenylalanine7α protons, as well as some 0.2-0.3 ppm shifts on parts of 2 phenylalanine ring systems. Almost all of these shifts decrease considerably with increasing temperature. Most of the observed NMR results are compatible with the properties of one family of low-energy conformations whose main features are a double βII bend Trp8-Lys9-, Thr10-Phe11, a close proximity of the trptophan8 and lysine9 side chains and an orientation of phenylalanine7 towards the phenylalanine6α,β protons. This set of conformations apparently forms a major contribution to the conformational equilibrium at room temperature. The properties of this

and

several other sets of low-energy conformations that do not dominate in aqueous solns. are discussed in relation to all available exptl. evidence.

L5 ANSWER 32 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1981:98096 CAPLUS

DN 94:98096

TI A proton nuclear magnetic resonance investigation of histidine-binding protein J of Salmonella typhimurium: a model for transport of L-histidine across cytoplasmic membrane

AU Ho, Chien; Giza, Yueh-Hua; Takahashi, Seizo; Ugen, Kenneth E.; Cottam, Patricia F.; Dowd, Susan R.  
CS Mellon Coll. Sci., Carnegie-Mellon Univ., Pittsburgh, PA, 15213, USA  
SO Journal of Supramolecular Structure (1980), 13(2), 131-45  
CODEN: JSPMAW; ISSN: 0091-7419  
DT Journal  
LA English  
AB High-affinity L-histidine transport in *S. typhimurium* requires the participation of a periplasmic binding protein (histidine-binding protein J) and 2 other proteins (P and Q proteins). High-resoln. 1H NMR spectroscopy at 600 MHz is used to investigate the conformations of this protein in the absence and presence of substrate. To gain a deeper insight into the nature of structural changes induced by histidine binding, deuterated phenylalanine or tyrosine was incorporated into the bacteria. 1H NMR spectra of selectively deuterated histidine-binding protein J were obtained and compared to the undeuterated protein. Several of the proton resonances have been assigned to the various aromatic amino acid residues of this protein. A model for the high-affinity transport of L-histidine across the cytoplasmic membrane of *S. typhimurium* is proposed. This model, a version of the pore model, assumes that both P and Q proteins are membrane bound and that the interface between these 2 proteins forms the channel for the passage of substrate. Histidine-binding protein J serves as the key for the opening of the channel for the passage of L-histidine. In the absence of substrate, this channel or gate is closed due to a lack of appropriate interactions among these 3 proteins. The channel can be opened on receiving a specific signal from the key; namely, the substrate-induced conformational changes in histidine-binding protein J. This model is consistent with available exptl. evidence for the high-affinity transport of L-histidine across the cytoplasmic membrane of *S. typhimurium*.

L5 ANSWER 33 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1980:639860 CAPLUS  
DN 93:239860  
TI Synthesis of stereoselectively deuterated phenylalanine and its use in conformational analysis of the side chain of phenylalanine residues in peptides  
AU Kobayashi, Junichi; Nagai, Ukon  
CS Lab. Organochem. Prep., Mitsubishi-Kasei Inst. Life Sci., Machida, 194, Japan  
SO Peptide Chemistry (1978), Volume Date 1977, 15th, 91-6  
CODEN: PECHDP; ISSN: 0388-3698  
DT Journal  
LA English  
AB Stereospecifically deuterated phenylalanine derivs. were prepared via asym. hydrolysis of deuterated phenylalanine esters by  $\alpha$ -chymotrypsin. Relative rotamer populations of deuterated H-Phe-NHMe, Ac-Phe-NHMe, and Ac-Phe-OH were studied by NMR spectroscopy in solvents of varying polarity. Side chain conformations in the phenylalanine derivs. are very sensitive to solvent polarity and solvent dependencies differ from each other. NMR anal. of 5-methionine-enkephalin containing a deuterated phenylalanine residue showed the presence of two gauche rotamers for the phenylalanine moiety.

L5 ANSWER 34 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1979:84171 CAPLUS  
DN 90:84171  
TI Studies in man using semi-tracer doses of deuterated phenylalanine and tyrosine: implications for the investigation of phenylketonuria using the deuterated phenylalanine load test  
AU Hoskins, J. A.; Pollitt, R. J.  
CS Univ. Dep. Psychiatry, Middlewood Hosp., Sheffield, UK  
SO Stable Isot., Proc. Int. Symp. (1978), Meeting Date 1977, 253-60.

Editor(s): Baillie, T. A. Publisher: Macmillan, London, Engl.

CODEN: 39QRAX

DT Conference

LA English

AB When L-tyrosine-2H (12.5 mg/kg orally) was given to normal subjects, the following 2H-labeled metabolites were detected in the urine: p-hydroxyphenylacetic acid, p-hydroxymandelic acid, and p-hydroxyphenyllactic acid. Simultaneous ingestion of L-tyrosine-2H (12.5 mg/kg) and L-phenylalanine-2H (25 mg/kg) resulted in the excretion of 2 more labeled metabolites, o- and m-hydroxyphenylacetic acids. The implications of these results in the detection of phenylketonuria are discussed.

L5 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1979:68256 CAPLUS

DN 90:68256

TI In vivo determination of phenylalanine hydroxylase activity using heptadeutero-phenylalanine and comparison to the in vitro assay values

AU Trefz, Friedrich K.; Bartholome, Klaus; Bickel, Horst; Lutz, Peter; Schmidt, Hildgund

CS Univ. Child. Hosp., Heidelberg, Fed. Rep. Ger.

SO Monographs in Human Genetics (1978), 9(Inborn Errors Metab. Man, Part 1, 1977), 108-13

CODEN: MOHGAD; ISSN: 0077-0876

DT Journal

LA English

AB Phenylalanine hydroxylase activity was determined in vivo by i.v. injection of heptadeutero L-phenylalanine and measuring the rate constant of elimination of deuterated phenylalanine from blood plasma as well as the concentration of deuterated tyrosine in plasma. The results were compared

with in vitro enzyme activities (needle liver biopsies) in hyperphenylalaninemic and phenylketonuric patients. The correlation coefficient was 0.95. The use of this assay in distinguishing hyperphenylalaninemic patients from phenylketonurics is discussed.

L5 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1978:187416 CAPLUS

DN 88:187416

TI In vivo studies of the phenylalanine-4-hydroxylase system in hyperphenylalaninemics and phenylketonurics

AU Curtius, H. C.; Zagalak, Maria Jolant; Baerlocher, K.; Schaub, J.; Leimbacher, W.; Redweik, U.

CS Dep. Pediatr., Univ. Zurich, Zurich, Switz.

SO Helvetica Paediatrica Acta (1978), 32(6), 461-9

CODEN: HPAAAE; ISSN: 0018-022X

DT Journal

LA English

AB In vivo phenylalanine-4-hydroxylase (EC 1.14.16.1) activity was determined in subjects loaded with deuterated L-phenylalanine-ds (200 mg/kg) by anal. of deuterated tyrosine and deuterated phenylalanine in plasma using mass fragmentog. Six phenylketonurics (PKU), 4 hyperphenylalaninemics, and 2 healthy controls were investigated. This method allowed a specific differentiation between PKU's, hyperphenylalaninemics and healthy controls. The hyperphenylalaninemic patients showed 7-17% of the phenylalanine-4-hydroxylase activity found in the 2 control persons. The PKU patients under diet showed 2-3% of the activity found in the control group. In the PKU patients, loaded while showing high phenylalanine blood concns. no activity could be measured.

L5 ANSWER 37 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1978:118381 CAPLUS

DN 88:118381

TI The labeling of urinary acids after oral doses of deuterated L-phenylalanine and L-tyrosine in normal subjects. Quantitative studies

with implications for the deuterated phenylalanine load test in phenylketonuria

AU Fell, Vanessa; Hoskins, John A.; Pollitt, Rodney J.  
CS Univ. Dep. Psychiatry, Middlewood Hosp., Sheffield, UK  
SO Clinica Chimica Acta (1978), 83(3), 259-69  
CODEN: CCATAR; ISSN: 0009-8981

DT Journal  
LA English

AB Oral doses of L-phenylalanine-2H5 (25 mg/kg) and L-tyrosine-2H2 (12.5 mg/kg) were given sep. to 3 normal subjects and together to a 4th subject. Blood samples were analyzed for deuterium-labeled phenylalanine and tyrosine, and urine for labeled o- and p-hydroxyphenylacetic, p-hydroxyphenyllactic, and p-hydroxymandelic acids. The labeling pattern of the urinary metabolites indicated that the para-compds. all originated in both hepatic and extrahepatic tissues. The plasma tyrosine did not appear to be in equilibrium with the tyrosine in the liver. A simple quant. relation between the labeling of these metabolites and the synthesis of labeled tyrosine from labeled phenylalanine in liver is apparently unlikely.

L5 ANSWER 38 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1978:62592 CAPLUS  
DN 88:62592

TI Studies on phenylalanine metabolism by use of tracer techniques.  
Synthesis and physicochemical features of L-phenylalanine[aromatic-d5]  
AU Tokuhisa, Sachiko; Yoshikawa, Haruhisa; Ichihara, Shigeyasu; Baba, Shigeo  
CS Kagawa Nutr. Coll., Tokyo, Japan  
SO Radioisotopes (1977), 26(9), 630-5  
CODEN: RAISAB; ISSN: 0033-8303

DT Journal  
LA Japanese

AB The title deuterium-labeled phenylalanine (I) was prepared in 18% yield from deuterium labeled benzaldehyde according to method of Herbst and Shemin. I according to IR and NMR spectra contained no detectable amount of H in its benzene ring. Mass spectrum of I is compared with that of L-phenylalanine.

L5 ANSWER 39 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1978:2543 CAPLUS  
DN 88:2543

TI Quantitation of deuterated and non-deuterated phenylalanine and tyrosine in human plasma using the selective ion monitoring method with combined gas chromatography-mass spectrometry. Application to the in vivo measurement of phenylalanine-4-monooxygenase activity

AU Zagalak, Maria Jolanta; Curtius, H. C.; Leimbacher, W.; Redweik, U.  
CS Univ. Paediatr. Dep., Kinderspital Zurich, Zurich, Switz.  
SO Journal of Chromatography (1977), 142, 523-31  
CODEN: JOCRAM; ISSN: 0021-9673

DT Journal  
LA English

AB A specific method is described for the quant. anal. of deuterated and nondeuterated phenylalanine and tyrosine in human plasma by gas chromatog.-mass spectrometry using selective ion monitoring. From the several derivs. investigated, the N- or N,O-trifluoroacetyl Me esters were the most suitable for this purposes. DL-Phenylalanine-4-d1 and L-tyrosine-d7 were used as internal stds. The sensitivity of this method permits the measurement of amts. as small as 2.5 ng/mL in plasma for both phenylalanine and tyrosine. The coeffs. of variation were 1.6% (n = 12) for phenylalanine and 3.0% (n = 12) for tyrosine. Using this method, an in vivo determination of phenylalanine 4-monooxygenase activity in humans is possible by loading the subjects with L-phenylalanine-d5 (deuterated in cell ring positions) and the subsequent measurement of L-tyrosine-d4 formed and residual L-phenylalanine-d5.

L5 ANSWER 40 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1977:117043 CAPLUS  
DN 86:117043  
TI Determination of deuterium-labeled phenylalanine and tyrosine in human plasma with high pressure liquid chromatography and mass spectrometry  
AU Trefz, Friedrich K.; Byrd, Dennis J.; Blaskovics, Milan E.; Kochen, Walter; Lutz, Peter  
CS Univ.-Kinderklin. Heidelberg, Heidelberg, Fed. Rep. Ger.  
SO Clinica Chimica Acta (1976), 73(3), 431-8  
CODEN: CCATAR; ISSN: 0009-8981  
DT Journal  
LA English  
AB A method is presented for the recovery of deuterated phenylalanine and tyrosine from human plasma. Phenylthiohydantoin derivs. are formed (Edman reaction) which are separated and isolated by high pressure liquid chromatog. The relative concentration of the deuterated amino acid is determined by mass spectrometry. The results obtained from a healthy person after oral loading with 40% monodeuterated L-phenylalanine are presented. The method appears to be suitable for in vivo studies of phenylalanine metabolism in humans.

L5 ANSWER 41 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1977:90209 CAPLUS  
DN 86:90209  
TI Simultaneous synthesis of both diastereomers of stereoselectively  $\beta$ -deuterated phenylalanines, (2S,3R)- and (2R,3R)-PhCHDCH(NH<sub>2</sub>)COOH  
AU Nagai, Ukon; Kobayashi, Junichi  
CS Mitsubishi-Kasei Inst. Life Sci., Tokyo, Japan  
SO Tetrahedron Letters (1976), (33), 2873-4  
CODEN: TELEAY; ISSN: 0040-4039  
DT Journal  
LA English  
AB A mixture of (2S,3R)-N-acetyl-L-phenylalanine-3-d<sub>1</sub> (I) and (2R,3R)-N-acetyl-D-phenylalanine-3-d<sub>1</sub> Et ester (II) was obtained in 6% overall yield from PhCDO by successive treatment with yeast, 4-Me-C<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>Cl, MeCOCH(Na)CO<sub>2</sub>Et, H<sup>+</sup>/HN<sub>3</sub>, and  $\alpha$ -chymotrypsin. The optical purities of I and II were 91 and 94%, resp. The epimeric purities were .apprx.92% at C-3.

L5 ANSWER 42 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1977:67973 CAPLUS  
DN 86:67973  
TI Synthesis of stereospecifically deuterated phenylalanines and determination of their configuration  
AU Bartl, Knut; Cavalar, Christiane; Krebs, Traute; Ripp, Engelbert; Retez, Janos; Hull, William E.; Guenther, Helmut G.; Simon, Helmut  
CS Inst. Org. Chem., Univ. Karlsruhe, Karlsruhe, Fed. Rep. Ger.  
SO European Journal of Biochemistry (1977), 72(2), 247-50  
CODEN: EJBCAI; ISSN: 0014-2956  
DT Journal  
LA English  
OS CASREACT 86:67973  
AB Starting from trans-cinnamic acid a chiral (-)-3-phenyl-propionic acid-2,3-2H was synthesized using Clostridium kluyveri cells as catalyst. The chiral dideuterated acid was converted by chemical methods to a mixture of (2R) and (2S)-phenyl-alanine-2,3-2H. By means of 1H-NMR spectroscopy and the action of D and L-amino-acid oxidase the configuration of the phenylalanine was shown to be (2R, 3S) and (2S, 3S), resp. The labeled phenylalanine is thus sterically and isotopically homogeneous at position 3 but heterogeneous at position 2.

L5 ANSWER 43 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1975:474238 CAPLUS

DN 83:74238  
TI Phenylalanine hydroxylase system in vivo. In vivo assay based on the liberation of deuterium or tritium into the body water from ring-labeled L-phenylalanine  
AU Milstien, Sheldon; Kaufman, Seymour  
CS Lab. Neurochem., Natl. Inst. Ment. Health, Bethesda, MD, USA  
SO Journal of Biological Chemistry (1975), 250(12), 4782-5  
CODEN: JBCHA3; ISSN: 0021-9258  
DT Journal  
LA English  
AB The rate of release of 2H into the body water from L-phenylalanine-2,3,4,5,6-2H5 was shown to be a valid measure of the activity of the phenylalanine hydroxylase system in vivo. At a dose of 0.5 g/kg, the rate of release of deuterons was linear for 60-90 min. Male rats, with 22-25% more phenylalanine hydroxylase activity in liver exts. than female rats, produced 2H from deuterated phenylalanine at a rate 20-30% greater than female rats. P-chlorophenylalanine, which irreversibly inhibited phenylalanine hydroxylase in vivo, caused a similar degree of inhibition of the rate of 2H formation as was found when phenylalanine hydroxylase was measured in exts. from the same group of animals. Methotrexate, which inhibited the phenylalanine hydroxylase system by preventing regeneration of the tetrahydropteridine cofactor, caused parallel inhibition of the in vivo assay as well as when the conversion of phenylalanine to tyrosine was measured in liver slices. Randomly ring-tritiated phenylalanine could be used interchangeably with ring-deuterated phenylalanine if greater sensitivity is needed in the in vivo assay for phenylalanine hydroxylase. However, a dose of 20-30  $\mu$ Ci/kg was required.

L5 ANSWER 44 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1975:58090 CAPLUS  
DN 82:58090  
TI Mono- and bideuterated L-phenylalanines  
AU Faulstich, H.; Trischmann, H.  
CS Abt. Chem., Max-Planck-Inst. Med. Forsch., Heidelberg, Fed. Rep. Ger..  
SO Analytical Biochemistry (1974), 62(2), 615-17  
CODEN: ANBCA2; ISSN: 0003-2697  
DT Journal  
LA English  
AB From the bromination products of L-phenylalanine, 2-bromo- and 4-bromophenylalanines, 2,3- 2,5-, and 3,4-dibromo-phenylalanines were obtained. Deuteration of these compds. on Pd-catalysts with either D gas or NaBD4 was studied in order to obtain L-phenylalanines which were labeled in the aromatic ring. Mass spectrometry indicated that the dideuterated compds. contained <10% of monodeuterated and <3% of nondeuterated phenylalanines. Monobrominated phenylalanines gave the deuterated derivs. with <3% of the H compound All the deuterated phenylalanines were optically pure.

L5 ANSWER 45 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1973:430164 CAPLUS  
DN 79:30164  
TI Use of deuterated phenylalanine for the elucidation of the phenylalanine-tyrosine metabolism  
AU Curtius, H. Ch.; Voellmin, J. A.; Baerlocher, K.  
CS Univ. Kinderklin, Kinderspital, Zurich, Switz.  
SO Org. Acidurias, Proc. Symp. Soc. Study Inborn Errors Metab., 9th (1972), 146-58. Editor(s): Stern, J. Publisher: Livingstone, Edinburgh, Scot.  
CODEN: 26SRAB  
DT Conference  
LA English  
AB Deuterium labeling was absent in p-hydroxyphenylpyruvic acid, p-hydroxyphenylacetic acid, p-hydroxyphenyllactic acid, and homovanillic acid and significantly reduced in m-hydroxyphenylacetic acid obtained from the urine of a phenylketonuria (PKU) patient orally loaded with 200 mg of

deuterated DL-phenylalanine (I)/kg body weight. The results confirm that the enzyme block in PKU cannot be circumvented. Similar deuterium labeling patterns were obtained with a hyperphenylalaninaemia patient, indicating that I is not being converted to tyrosine (II). The concentration of the I metabolites were significantly lower in this patient before and during the loading test, suggesting another pathway for I degradation exists in hyperphenylalaninaemia patients. Deuterated hippuric acid was not detected with either of the patients or the normal subject indicating that it is not synthesized through the phenylalanine-tyrosine pathway. Deuterated mandelic acid was detected in the urine of each subject identifying it as a normal product of I metabolism.

L5 ANSWER 46 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1972:109947 CAPLUS

DN 76:109947

TI Use of deuterated phenylalanine for the elucidation of phenylalanine-tyrosine metabolism

AU Curtius, H. Ch.; Voellmin, J. A.; Baerlocher, K.

CS Kinderspital, Univ. Zurich, Zurich, Switz.

SO Clinica Chimica Acta (1972), 37, 277-85

CODEN: CCATAR; ISSN: 0009-8981

DT Journal

LA English

AB The in vivo use of stable isotopes, e.g.,  $2H$ , for the study of metabolic pathways is demonstrated with the example of phenylalanine-tyrosine metabolism. A healthy child, a patient with phenylketonuria, and a patient with hyperphenylalaninemia were loaded with 200 mg deuterated phenylalanine/kg. The concentration and  $2H$  content of the excreted aromatic acids were examined by gas chromatog. and gas chromatog.-mass spectrometry. Unlike the case in the healthy child, no  $2H$  was incorporated into the metabolites of tyrosine by the patients with phenylketonuria and hyperphenylalaninemia. The meta-hydroxylation of phenylalanine, leading to m-hydroxyphenylacetic acid, was blocked during the loading test in phenylketonuric as well as in hyperphenylalaninemic patients.

L5 ANSWER 47 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1971:487047 CAPLUS

DN 75:87047

TI Biosynthesis of dithiadiketopiperazine antibiotics: comparison of possible aromatic amino acid precursors

AU Brannon, D. R.; Mabe, J. A.; Molloy, B. B.; Day, W. A.

CS Lilly Res. Lab., Eli Lilly and Co., Indianapolis, IN, USA

SO Biochemical and Biophysical Research Communications (1971), 43(3), 588-94

CODEN: BBRC9; ISSN: 0006-291X

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB Phenylalanine was a more efficient precursor than tyrosine for the production of gliotoxin (I) by *Penicillium terlikowskii* or *Trichoderma viride*, as well as for the production of bisdethiodi(methylthio)acetylaranotin (II) by *Arachniotus aureus*. All of the aromatic and both of the methylene deuteriums of deuterated phenylalanine were retained upon incorporation into acetylaranotin by *Aspergillus terreus*.

L5 ANSWER 48 OF 48 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1965:407600 CAPLUS

DN 63:7600

OREF 63:1345c-d

TI Infrared spectra and vibration assignment of DL-phenylalanine

AU Garrigou-Lagrange, Chantal; Dupuy, Bernard; Josien, Marie Louise

CS Fac. Sci., Bordeaux, Fr.

SO Journal de Chimie Physique et de Physico-Chimie Biologique (1965), 62(3), 265-72

CODEN: JCPBAN; ISSN: 0021-7689

DT Journal  
LA French  
AB The ir spectrum of DL-phenylalanine was measured, 400-3500 cm.<sup>-1</sup> Band assignments were made by analogy with the spectra of phenylalanine-HCl, Na phenylalaninate, N-deuterated phenylalanine, PhMe, PhEt, and  $\beta$ -phenylpropionic acid. Some normal vibrations were found: 27 of Ph, 12 of -C $\beta$ -C $\alpha$ CN; 9 valence or deformation vibrations of CH links to the chain -CH<sub>2</sub>-CH; 9 vibrations of NH<sub>3</sub><sup>+</sup>; and 6 of COO<sup>-</sup>.

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	153.33	153.54
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-37.44	-37.44

STN INTERNATIONAL LOGOFF AT 18:02:53 ON 08 FEB 2007